

# Entanglement of a microcanonical ensemble

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## Abstract

We replace time-averaged entanglement by ensemble-averaged entanglement and derive a simple expression for the latter. We show how to calculate the ensemble average for a two-spin system and for the Jaynes-Cummings model. In both cases the time-dependent entanglement is known as well so that one can verify that the time average coincides with the ensemble average.

## 1 Introduction

The entanglement of particles is in principle a time-dependent quantity. This time-dependence has been analysed recently in chaotic systems [1], in experimental spectra of triatomic molecules [2], and in Rydberg atoms [3]. Time-dependent entanglement has been studied in theoretical models, like the Dicke model [4], a model of coupled kicked tops [5], the Harper Hamiltonian [6], a dimer model [7], Bose-Einstein condensates [8]. In these papers, the notions of time-averaged entanglement and ensemble-averaged entanglement have been shown to be useful in monitoring phase transitions, although the generality of this relationship has been questioned, see e.g. [3].

In addition, time-averaged and ensemble-averaged entanglement are conserved quantities of quantum microcanonical ensembles [9]. As such they are of interest in the study of closed systems. This context is suited to discuss the relation between both concepts, and is the starting point of the present paper.

The entanglement of formation of a pure state is taken here to be defined as the von Neumann entropy of the reduced density matrix. Often, the von Neumann entropy is replaced by the linear entropy because the latter can be computed more easily. In the present paper the use of the linear entropy is essential to obtain simple results.

For the sake of completeness, and to fix notations, the definitions of entanglement of pure and of mixed states are reproduced in the next section. Section

3 introduces the entanglement of microcanonical ensembles of wavefunctions. The main result is announced in Section 4. The proof is found in the Appendix. It is followed by a section devoted to the complications that arise when the state of the system has additional symmetries. In Sections 6 and 7 the main result is applied to a system of two interacting spins. Section 8 deals with the Jaynes-Cummings model. For this model the time-dependent entanglement is known so that it can be compared with the ensemble average. A short discussion follows in Section 9.

## 2 Definition of entanglement

Consider two independent subsystems, labelled A and B. With each normalised wavefunction  $\psi$  of the combined system corresponds a reduced density matrix  $\rho_A$  of the subsystem labelled A. The latter is defined by the relation

$$\text{Tr}_A \rho_A X = \langle \psi | X \otimes \mathbb{I} | \psi \rangle \quad \text{for all } X. \quad (1)$$

The entanglement of  $\psi$  is then equal to the von Neumann entropy of  $\rho_A$ . For technical reasons we replace this entropy by the linear entropy. The general definition of entanglement is

$$\mathcal{E}_A(\psi) = S_f(\rho_A) \equiv \text{Tr}_A \rho_A f(\rho_A), \quad (2)$$

with  $f(x) = -\ln x$  in the von Neumann case, and  $f(x) = 1 - x$  in the case of the linear entropy.

If  $\psi$  is of the product form  $\psi = \psi_A \otimes \psi_B$  then  $\rho_A$  is a one-dimensional projection operator. Hence, the entanglement vanishes. A similar definition holds for  $\rho_B$  and for  $\mathcal{E}_B$ . The entanglements  $\mathcal{E}_A(\psi)$  and  $\mathcal{E}_B(\psi)$  are equal [10]. To see this, select a basis  $u_m$  in subsystem A and a basis  $v_p$  in subsystem B, so that

$$\psi = \sum_n \sqrt{p_n} u_n \otimes v_n. \quad (3)$$

This is possible by means of the Schmidt construction. Then  $\rho_A$  and  $\rho_B$  are diagonal, with eigenvalues  $p_n$ , and with entropy equal to  $\sum_n p_n f(p_n)$ .

Often, the state of the system is not described by a wavefunction  $\psi$  but by a density matrix  $\rho$ . Such a density matrix can be written into the form

$$\rho = \sum_n p_n |\psi_n\rangle \langle \psi_n|, \quad (4)$$

with  $p_n \geq 0$ ,  $\sum_n p_n = 1$ , and with  $\psi_n$  normalised wavefunctions. Then the entanglement of  $\rho$  has been defined [11] as the minimum of the average entanglement

$$\mathcal{E}(\rho) = \min \sum_n p_n \mathcal{E}_A(\psi_n), \quad (5)$$

where the minimum is taken over all possible ways to write (4).

### 3 Definition of mean entanglement of a microcanonical ensemble

The mean entanglement, which is studied in the present paper, is *not* the average (5), but rather the average over a microcanonical ensemble, as introduced in [9].

Let be given a density matrix  $\rho$ , which is diagonal in the orthonormal basis of wavefunctions  $\psi_n$ , with eigenvalues  $p_n$ :  $\rho\psi_n = p_n\psi_n$ . Associated with this diagonal density matrix is an ensemble of wavefunctions of the form

$$\psi = \sum_n \sqrt{p_n} e^{i\chi_n} \psi_n, \quad (6)$$

where the  $\chi_n$  are arbitrary phase factors. The ensemble average of the entanglement is then denoted  $\bar{\mathcal{E}}$  and is given by

$$\bar{\mathcal{E}} = \left\langle \mathcal{E}_A \left( \sum_n \sqrt{p_n} e^{i\chi_n} \psi_n \right) \right\rangle_\chi, \quad (7)$$

where the average over  $\chi$  is obtained by integrating over all phase factors  $\chi_n$  from 0 to  $2\pi$ , normalised by dividing by a factor  $2\pi$ . Note that the ensemble average (7) does not depend on the chosen subsystem because  $\mathcal{E}_A(\psi) = \mathcal{E}_B(\psi)$  for all  $\psi$ .

The ensemble (6) can be obtained by starting from a single wavefunction  $\psi$ , in combination with the quantum mechanical time evolution. The Hamiltonian  $H$  is the generator of the unitary time evolution

$$\psi_t = U(t)\psi \quad \text{with} \quad U(t) = e^{-i\hbar^{-1}tH}. \quad (8)$$

The time average of the entanglement  $\mathcal{E}_A(\psi)$  is then defined by

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathcal{E}_A(\psi_t). \quad (9)$$

Assume now that the Hamiltonian is diagonal in the basis of wavefunctions  $\psi_n$ , with eigenvalues  $\epsilon_n$ . Then one has

$$\psi_t = \sum_n \lambda_n e^{-i\hbar^{-1}\epsilon_n t} \psi_n \quad (10)$$

and hence

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \mathcal{E}_A \left( \sum_n \lambda_n e^{-i\hbar^{-1}\epsilon_n t} \psi_n \right). \quad (11)$$

The wavefunctions  $\psi_t$  belong to the ensemble (6) with  $p_n = |\lambda_n|^2$ . If the conditions of the classical ergodic theorem holds then the time average (11) coincides with the ensemble average (7) — see [9]. But even when the classical ergodic theorem does not hold one can continue to use the ensemble average instead of the time average because experimentally the slightest perturbation may restore ergodicity.

## 4 Main result

Let be given an ensemble of wavefunctions of the form (6). With each of the basis vectors  $\psi_n$  is associated a couple of reduced density matrices  $\rho_A$  and  $\rho_B$ . For convenience, these will be denoted  $\sigma_n$  and  $\tau_n$ . Introduce the density matrices  $\sigma$  and  $\tau$ , defined by

$$\sigma = \sum_n p_n \sigma_n \quad \text{and} \quad \tau = \sum_n p_n \tau_n. \quad (12)$$

In some sense,  $\sigma$  is the ensemble average of  $\rho_A$ ,  $\tau$  is the ensemble average of  $\rho_B$ .

Our main result is now that the mean entanglement, defined by (7), using the linear entropy  $S_1$ , can be written as

$$\overline{\mathcal{E}} = S_1(\sigma) + S_1(\tau) - \Delta, \quad (13)$$

where  $\Delta$  is a contribution common to both  $S_1(\sigma)$  and  $S_1(\tau)$ . It is given by

$$\Delta = 1 - \sum_m p_m^2 \text{Tr}_A \sigma_m^2 = 1 - \sum_m p_m^2 \text{Tr}_B \tau_m^2. \quad (14)$$

The proof of this relation is given in the Appendix.

The applications of (13) are explored in later sections.

## 5 Degeneracies

The ensemble (6) is uniquely defined by the density operator  $\rho$  in the case that the eigenvalues  $p_n$  of  $\rho$  are two-by-two distinct. Then the eigenfunctions  $\psi_n$  are unique up to a phase factor. However, If some of the eigenvalues  $p_n$  coincide then the orthonormal basis is non-unique. In particular, if a non-zero eigenvalue  $p_n$  is degenerate then different choices of orthonormal wavefunctions may influence the value of  $\overline{\mathcal{E}}$ . This shows that  $\overline{\mathcal{E}}$  is the average entanglement of the ensemble and is not suitable as a definition of the entanglement of  $\rho$ .

A similar question is whether the entanglement of the ensemble can be used as the definition of the mean entanglement of the wavefunction  $\psi$ . Consider the situation that some of the eigenvalues  $\epsilon_n$  of the Hamiltonian  $H$  are degenerate. Then the basis of wavefunctions  $\psi_n$ , which diagonalises  $H$ , is not uniquely defined (up to phase factors). In that case the wavefunction  $\psi$  should not be decomposed into an arbitrary diagonalising orthonormal basis. Rather, it should be projected onto the invariant subspaces of  $H$ . This determines in a unique way an orthonormal basis which then can be used to form the ensemble associated with  $\psi$ . An example of the degenerate case follows below.

## 6 Two-spin example

The simplest example is that of two quantum spins, each described by Pauli spin matrices, and a Hamiltonian  $H$  which is diagonal in the basis of wavefunctions

$$\begin{aligned}\psi_1 &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\ \psi_2 &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \\ \psi_3 &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ \psi_4 &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle).\end{aligned}\tag{15}$$

We assume that the energy levels are non-degenerate. Their actual value is not needed.

The reduced density matrices  $\sigma_m$  and  $\tau_m$ , corresponding with  $\psi_m$ , are all equal to  $\frac{1}{2}\mathbb{I}$ . Hence, also the averages  $\sigma$  and  $\tau$  are equal to  $\frac{1}{2}\mathbb{I}$ . As a consequence, the linear entropies  $S_1(\sigma)$  and  $S_1(\tau)$  both equal  $1/2$ . However, the common part  $\Delta$  depends on the choice of wavefunction  $\psi$ . One finds

$$\Delta = 1 - \sum_m p_m^2 \text{Tr}_A \sigma_m^2 = 1 - \frac{1}{2} \sum_m p_m^2.\tag{16}$$

The final result for the mean entanglement of  $\psi$  is therefore

$$\bar{\mathcal{E}} = \frac{1}{2} + \frac{1}{2} - \left(1 - \frac{1}{2} \sum_m p_m^2\right) = \frac{1}{2} \sum_m p_m^2.\tag{17}$$

Note that this result lies between  $1/4$  and  $1/2$ .

It is possible but tedious to verify by explicit calculation that the mean entanglement (17) coincides with the time average of  $\mathcal{E}_A(\psi_t)$ , as it should be.

## 7 Degenerate two-spin example

Consider a two-spin system with energy  $-\epsilon$  for anti-parallel spins and  $+\epsilon$  for parallel spins. This is a degenerate limit of the previous example. The ensemble, generated by an arbitrary  $\psi$ , now contains two free phase factors instead of four. It consists of all wavefunctions of the form

$$e^{i\chi_1} \lambda_1 \psi_1 + e^{i\chi_2} \lambda_2 \psi_2\tag{18}$$

with  $\chi_1$  and  $\chi_2$  arbitrary, and with  $\lambda_1 \psi_1, \lambda_2 \psi_2$  given by

$$\begin{aligned}\lambda_1 \psi_1 &= |\uparrow\downarrow\rangle \langle\uparrow\downarrow|\psi\rangle + |\downarrow\uparrow\rangle \langle\downarrow\uparrow|\psi\rangle \\ \lambda_2 \psi_2 &= |\uparrow\uparrow\rangle \langle\uparrow\uparrow|\psi\rangle + |\downarrow\downarrow\rangle \langle\downarrow\downarrow|\psi\rangle.\end{aligned}\tag{19}$$

The coefficients  $\lambda_1$  and  $\lambda_2$  are chosen in such a way that  $\psi_1$  and  $\psi_2$  are normalised. The reduced density matrices are found to be

$$\begin{aligned} p_1 \sigma_1 &= \begin{pmatrix} p_{+-} & 0 \\ 0 & p_{-+} \end{pmatrix} \\ p_2 \sigma_2 &= \begin{pmatrix} p_{++} & 0 \\ 0 & p_{--} \end{pmatrix}, \end{aligned} \quad (20)$$

with  $p_{+-} = |\langle \uparrow \downarrow | \psi \rangle|^2$  and similar definitions for  $p_{-+}$ ,  $p_{++}$  and  $p_{--}$ . Similar expressions hold for  $\tau_1$  and  $\tau_2$

$$\begin{aligned} p_1 \tau_1 &= \begin{pmatrix} p_{-+} & 0 \\ 0 & p_{+-} \end{pmatrix} \\ p_2 \tau_2 &= \begin{pmatrix} p_{++} & 0 \\ 0 & p_{--} \end{pmatrix}. \end{aligned} \quad (21)$$

The mean entanglement can now be calculated using (13). The result is

$$\overline{\mathcal{E}} = 2p_{++}p_{--} + 2p_{+-}p_{-+}. \quad (22)$$

In the notation of the previous section this becomes

$$\overline{\mathcal{E}} = \frac{1}{2}(p_1 - p_2)^2 + \frac{1}{2}(p_3 - p_4)^2, \quad (23)$$

which is less than (17) by the term  $-p_1p_2 - p_3p_4$ .

## 8 The Jaynes-Cummings model

The Jaynes-Cummings model [12, 13] describes a two-level system interacting with a harmonic oscillator. The latter represents a single mode of the electromagnetic field in a cavity. The model has been studied extensively.

The Hamiltonian of the model reads

$$H = \hbar\omega a^\dagger a + \frac{1}{2}\hbar\omega_0\sigma_z + \hbar\kappa(a^\dagger\sigma_- + a\sigma_+), \quad (24)$$

with  $a^\dagger$  and  $a$  creation and annihilation operators of the harmonic oscillator, and with the Pauli matrices  $\sigma_z$  and  $\sigma_\pm$  describing the two-level system.

Let  $|g\rangle$  and  $|e\rangle$  denote the ground state, respectively the excited state of the two-level system. Let  $|n\rangle$ ,  $n = 0, 1, \dots$  denote the eigenstates of the harmonic oscillator. The eigenstates of the Jaynes-Cummings Hamiltonian are explicitly known, see e.g. [14]. An orthonormal basis of eigenfunctions is given by

$$\begin{aligned} \psi_0 &= |g\rangle \otimes |0\rangle \\ \psi_{1,n} &= \cos(\theta_n)|g\rangle \otimes |n+1\rangle + \sin(\theta_n)|e\rangle \otimes |n\rangle \\ \psi_{2,n} &= -\sin(\theta_n)|g\rangle \otimes |n+1\rangle + \cos(\theta_n)|e\rangle \otimes |n\rangle. \end{aligned} \quad (25)$$

The angles  $\theta_n$ ,  $n = 0, 1, 2, \dots$  follow from the relation

$$\tan \theta_n = \kappa \frac{\sqrt{n+1}}{\frac{1}{2}(\omega - \omega_0) + \lambda_n} \quad (26)$$

with

$$\lambda_n = \sqrt{\frac{1}{4}(\omega - \omega_0)^2 + \kappa^2(n+1)}. \quad (27)$$

The time-dependence of the reduced density matrix can be calculated explicitly if the initial state is a product state with the two-level system in the excited state and the harmonic oscillator is in the  $n$ -th eigenstate, see e.g. [14]. The result for the reduced state of the two-level system is

$$\rho_A(t) = W_n(t)|g\rangle\langle g| + (1 - W_n(t))|e\rangle\langle e| \quad (28)$$

with

$$W_n(t) = 2\gamma_n \sin^2(t\kappa\sqrt{n+1}) \quad (29)$$

and with

$$\gamma_n = \frac{1}{2} \sin^2(2\theta_n). \quad (30)$$

The linear entanglement is therefore

$$\mathcal{E}_A(\psi_t) = 1 - W_n^2(t) - (1 - W_n(t))^2. \quad (31)$$

The time average equals

$$\langle \mathcal{E}_A(\psi_t) \rangle_t = 2\gamma_n - 3\gamma_n^2. \quad (32)$$

It is straightforward to calculate the reduced density matrices for the eigenfunctions of the model. The result is

$$\sigma_0 = |0\rangle\langle 0|, \quad (33)$$

$$\sigma_{1,n} = \cos^2 \theta_n |n+1\rangle\langle n+1| + \sin^2 \theta_n |n\rangle\langle n|, \quad (34)$$

$$\sigma_{2,n} = \sin^2 \theta_n |n+1\rangle\langle n+1| + \cos^2 \theta_n |n\rangle\langle n|, \quad (35)$$

$$\tau_0 = |g\rangle\langle g|, \quad (36)$$

$$\tau_{1,n} = \cos^2 \theta_n |g\rangle\langle g| + \sin^2 \theta_n |e\rangle\langle e|, \quad (37)$$

$$\tau_{2,n} = \sin^2 \theta_n |g\rangle\langle g| + \cos^2 \theta_n |e\rangle\langle e|. \quad (38)$$

Hence, it is straightforward to evaluate the mean entanglement  $\overline{\mathcal{E}}$  for an arbitrary wavefunction  $\psi$ . However, we did not succeed to rewrite the resulting expression in a simple and transparent way.

In the case that  $\psi$  is of the product form

$$\psi = |e\rangle \otimes |n\rangle = \sin(\theta_n)\psi_{1,n} + \cos(\theta_n)\psi_{2,n} \quad (39)$$

one obtains

$$\begin{aligned}
\sigma &= \sin^2(\theta_n)\sigma_{1,n} + \cos^2(\theta_n)\sigma_{2,n} \\
&= \gamma_n|n+1\rangle\langle n+1| + (1-\gamma_n)|n\rangle\langle n| \\
\tau &= \sin^2(\theta_n)\tau_{1,n} + \cos^2(\theta_n)\tau_{2,n} \\
&= \gamma_n|g\rangle\langle g| + (1-\gamma_n)|e\rangle\langle e| \\
\Delta &= 1 - \sin^4(\theta_n)\text{Tr}_B\tau_{1,n}^2 - \cos^4(\theta_n)\text{Tr}_B\tau_{2,n}^2 \\
&= 1 - (1-\gamma_n)^2.
\end{aligned} \tag{40}$$

This leads to the result

$$\bar{\mathcal{E}} = 2\gamma_n - 3\gamma_n^2, \tag{41}$$

which is identical with the time-averaged result (32).

## 9 Discussion

The calculation of the time-dependence of the entanglement of a quantum system is a hard problem. The average over time is more accessible because it can be replaced by an ensemble average. This is in particular so when the entanglement is defined using the linear entropy instead of the von Neumann entropy of the reduced density matrix, because in that case there exists a simple expression for the mean entanglement — see (13). We have used this expression in a two-spin system and in the Jaynes-Cummings model. For these systems it is feasible to calculate both the averages over time and over the ensemble of wavefunctions. The results of the two calculations coincide, as it should be.

We have pointed out that a systematic degeneracy of the energy levels of the Hamiltonian due to the presence of a symmetry influences the choice of the ensemble of wavefunctions, used in the calculation of the average entanglement. In the example of the two spin system the additional symmetry leads to a reduction of the entanglement.

Finally let us note that the use of the linear entropy is rather essential in our paper. It is of course possible as well to define the ensemble average of the entanglement, based on the von Neumann entropy. It is however unlikely that a simple formula like (13) exists in that case.

## Appendix

Here, the proof of (13) is given. From the definition (7) follows, assuming a linear entropy,

$$\bar{\mathcal{E}} = 1 - \langle \text{Tr}_A \rho_A^2(\chi) \rangle_\chi, \tag{42}$$

with  $\rho_A(\chi)$  defined by

$$\text{Tr}_A \rho_A(\chi) X = \left\langle \sum_m \sqrt{p_m} e^{i\chi_m} \psi_m \middle| X \otimes \mathbb{I} \middle| \sum_n \sqrt{p_n} e^{i\chi_n} \psi_n \right\rangle$$



$$= \sum_{mn} \sqrt{p_m p_n} e^{-i(\chi_m - \chi_n)} \text{Tr}_A \sigma_{mn} X \quad (43)$$

with  $\sigma_{mn}$  defined by

$$\text{Tr}_A \sigma_{mn} X = \langle \psi_m | X \otimes \mathbb{I} | \psi_n \rangle. \quad (44)$$

Hence, one obtains

$$\begin{aligned} \bar{\mathcal{E}} &= 1 - \left\langle \text{Tr}_A \left( \sum_{mn} \sqrt{p_m p_n} e^{-i(\chi_m - \chi_n)} \sigma_{mn} \right)^2 \right\rangle_\chi \\ &= 1 - \sum_{mn} \sum_{rs} \sqrt{p_m p_n p_r p_s} \left\langle e^{-i(\chi_m - \chi_n)} e^{-i(\chi_r - \chi_s)} \right\rangle_\chi \text{Tr}_A \sigma_{mn} \sigma_{rs} \\ &= 1 - \sum_{mn} p_m p_n \text{Tr}_A \sigma_{mm} \sigma_{nn} - \sum_{mn} p_m p_n \text{Tr}_A \sigma_{mn} \sigma_{nm} \\ &\quad + \sum_m p_m^2 \text{Tr}_A \sigma_{mm}^2. \end{aligned} \quad (45)$$

Now use that  $\sigma_{mm} \equiv \sigma_m$  to see that the first two terms yield the contribution  $S_1(\sigma)$ . The last term is  $1 - \Delta$ . Hence, it remains to be shown that

$$S_1(\tau) = 1 - \sum_{mn} p_m p_n \text{Tr}_A \sigma_{mn} \sigma_{nm}. \quad (46)$$

Choose an orthonormal basis  $u_r$  for the subsystem A and an orthonormal basis  $v_p$  for the subsystem B. Then one has

$$\sigma_{mn} = \sum_{rsp} [\langle \psi_m | u_s \otimes v_p \rangle \langle u_r \otimes v_p | \psi_n \rangle] |r\rangle \langle s| \quad (47)$$

so that

$$\begin{aligned} \text{Tr}_A \sigma_{mn} \sigma_{nm} &= \sum_{rspq} \langle \psi_m | u_s \otimes v_p \rangle \langle u_r \otimes v_p | \psi_n \rangle \\ &\quad \times \langle \psi_n | u_r \otimes v_q \rangle \langle u_s \otimes v_q | \psi_m \rangle \\ &= \sum_{pq} \langle \psi_m | (\mathbb{I} \otimes |v_p\rangle \langle v_q|) | \psi_m \rangle \langle \psi_n | (\mathbb{I} \otimes |v_q\rangle \langle v_p|) | \psi_n \rangle \\ &= \sum_{pq} \langle v_q | \tau_m | v_p \rangle \langle v_p | \tau_n | v_q \rangle \\ &= \text{Tr}_B \tau_m \tau_n. \end{aligned} \quad (48)$$

The relation (46) now follows readily.

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